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IN THE CRANKED HFB MODEL

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Abstract. A number of smoothly behaving configurations within the $i_{13/2}$ shell has been constructed by eliminating the interaction between certain quasiparticle levels near the Fermi surface. Using these configurations we have investigated how the size of the pairing gap is influenced by an increasing rotational frequency and by particle number projection. The special problems connected with the treatment of configuration changes in the HFB-model have been studied in some detail, taking the behaviour of the smooth configurations as a reference.



1. INTRODUCTION

In a large number of papers (see e.g. ref. ^{1,2}) for a relevant list of references) during the last ten years the pairing properties of rotating nuclei have been investigated using various models, extending from schematic few-level models to full scale calculations for heavy nuclei. Although the explicit formulation thus might be quite different, a common feature of most of these models is that they are based on the cranking concept, which is also the case in this work. If such calculations are performed self-consistently, it is quite often found that the pairing gap, $\Delta_{s.c.}$, steeply decreases at a quite well-defined cranking frequency, ω_c . (See e.g. refs. ^{3,4}.) If the decrease is sufficiently steep, it might lead to a situation where the rotational frequency locally decreases although the angular momentum increases, thus giving a possible explanation of backbending. However, recent investigations ^{5,6}) indicate that the backbending is caused by the crossing of the ground band (g-band) with an aligned 2-quasiparticle band (s-band). The observed aligned angular momentum, i , of the s-band and the crossing frequency ⁵) can most easily be understood if it is assumed that the pairing gap is large, almost comparable to that of the ground state, (see fig. 1) for both the crossing bands, which is in obvious contradiction to the self-consistent calculations referred to above.

It is well-known that the introduction of pair correlations, following the HFB-concept ⁷), violates the conservation of particle number. This deficiency can relatively easily be removed by performing particle number projection ⁸). It is then found that the change in $\Delta_{s.c.}$ in the backbending region is considerably reduced ⁹). In particular, the gap of the s-band remains large. It should be noted that a literal use of the cranked HFB-model requires a sudden reduction of $\Delta_{s.c.}$ in order to explain backbending ⁴). However, this is not the case in the approach taken in ref. ⁵). On the contrary, it is there assumed that the change in $\Delta_{s.c.}$ is small enough to be neglected in a first approximation.

From the above considerations it seems obvious that the particle number projection is essential in order to obtain reliable results from the cranked HFB-model. Therefore, we shall in this paper investigate the influence of particle number projection on the size of the pairing gap. We shall also discuss how the size of the gap is affected by an increasing rotational frequency and by configuration changes.

As a matter of fact, the cranking model is by far the simplest fully microscopic model for describing high-spin states. One may therefore expect it to be in use for still a long time, although it has quite often been criticized. It is true that it contains, in addition to what has been discussed above, still a number of less appealing features. Thus e.g. the cranking wave functions show a great spread in angular momentum ¹⁰⁾, especially in the backbending region, and the description of band crossings remains a delicate question, since the cranking model describes an interaction at a fixed frequency, while the actual interaction between rotational bands takes place between states with the same angular momentum. However, analysis of a large number of experimental data ¹¹⁾ have shown that the cranked HFB-model describes, with good accuracy, the observed quasiparticle excitation energies as well as the amount of aligned angular momentum. It also gives very useful qualitative predictions about the interaction strength between different rotational bands, which determines the occurrence of backbending. Hence, the cranked HFB-model has a lot of predictive power, and a detailed investigation in order to understand the deficiencies of the model is strongly motivated, since an uncritical use may easily give rise to misleading conclusions, and may even put the usefulness of the model in question.

To facilitate the understanding of certain features of the cranked HFB-model, we have in this work introduced a set of non-interacting quasiparticle levels (see section 2). The ground state configuration, defined in terms of these levels, corresponds to the 'reference configuration', introduced in ref. ¹¹⁾. It plays an essential role in the analysis of experimental data and a theoretical study of its properties would be very useful.

2. THE SOLUTION OF THE HFB-EQUATIONS

In this paper, as in several other papers ^{4,12,13)}, treating related problems, we restrict ourselves to a model space consisting of a pure $i_{13/2}$ shell. This space is, however, sufficiently large to allow a qualitative discussion of those low-lying bandcrossings which are responsible for most of the observed backbendings in the rare-earth region. An exception is the proton backbending around $I \approx 28 \hbar$, which, however, can be treated in an analogous way using the $h_{11/2}$ shell.

We may then write our Hamiltonian as

$$H = \sum_m (e_m - \lambda) a_m^\dagger a_m - \omega \sum_{m,n} \langle m | j_x | n \rangle a_m^\dagger a_n - \Delta \sum_m (a_m^\dagger a_{\bar{m}}^\dagger + a_{\bar{m}} a_m), \quad (2.1)$$

where the single-particle energies are given by

$$e_m = \kappa \frac{3m^2 - j(j+1)}{j(j+1)} + e_0. \quad (2.2)$$

The constant e_0 is of no importance for the solutions and may be chosen as zero. However, for certain applications a non-zero value is more convenient (see section 7). By choosing $\kappa=0.392 \hbar\omega_0$ (and $e_0=6.655 \hbar\omega_0$) we reproduce the Nilsson neutron levels at the deformation $\epsilon=0.27$, $\epsilon_4=0.02$, corresponding roughly to the ground state of ^{168}Er , within one pro mille. This gives a certain realism to the model, at least as far as the quasiparticle energies are concerned (see fig. 2, which may be compared to fig. 1 of ref. ¹¹⁾). The neglect of the negative parity states near the Fermi surface can, however, only partly be compensated for by increasing the pairing strength, G , of eq. (3.1). The model therefore only gives a qualitative description, so the calculated values of the gap, the crossing frequencies etc. should not be compared directly with the experimental values.

Since we shall occasionally give explicit expressions for the wave functions, we have to define our basis states. These have been chosen as

$$|\bar{m}\rangle = \frac{1}{\sqrt{2}} \{ |66 \frac{13}{2} m\rangle + |66 \frac{13}{2} -m\rangle \} \quad \text{having } \alpha=1/2$$

and (2.3)

$$|m\rangle = \frac{1}{\sqrt{2}} \{ |66 \frac{13}{2} m\rangle - |66 \frac{13}{2} -m\rangle \} \quad \text{having } \alpha=-1/2$$

where α is the signature as defined in ref. ^{11,14)} and m takes the values $1/2, 3/2, \dots, 13/2$. The states $|N=6, \ell=6, j=13/2, \pm m\rangle$ form the full set of basis states for the $i_{13/2}$ shell.

The solution of the HFB-equations can most conveniently be displayed as quasiparticle energy diagrams as in fig. 2. For the detailed interpretation of such a diagram we refer to ref. ¹¹⁾.

It is well-known that in the vicinity of those frequencies where two quasiparticle levels repel each other due to a weak interaction (e.g. at ω_1

in fig. 2), the HFB-calculations are not reliable, if one of the levels is occupied and the other is free. As discussed in ref. ¹¹⁾ this deficiency can be overcome by connecting through the crossing the levels with the same character, i.e. reconstructing the non-interacting levels. This leads to a sharp crossing between the corresponding rotational bands which, however, is a less severe drawback, especially if the interaction is weak (see e.g. ref. ¹⁵⁾) and it can be compensated afterwards by introducing an interaction between the bands as discussed in ref. ¹²⁾.

Because the occurrence of weak interactions has a very dramatic influence on the self-consistent pairing gap, we have in this work reconstructed the non-interacting levels, as shown in fig. 3. This allows us to study the properties of an individual configuration up to very high frequencies without any disturbances from the level crossings. In practice the elimination of the interaction at the level crossings requires serious attention, since in general the individual crossings cannot be treated separately. Thus, e.g., if the first interaction (at ω_1) is not extremely weak, it still has a considerable influence on the energies in the region of the second interaction around ω_2 . Furthermore, a relatively high accuracy is needed in the determination of the crossing frequencies in order to get well-behaved non-interacting wave functions in the crossing regions. The quality of the wave functions can be tested by calculating e.g. the expectation value $\langle j_x \rangle$, which has to behave smoothly in the crossing region. For a more detailed description we refer to a forthcoming publication ¹⁶⁾. Some further remarks are also given in section 4.

The low-lying excitations, which we shall discuss in this paper involve only levels near the Fermi surface. These levels are labelled a, b, c, ... if above and -a, -b, -c, ... if below the Fermi energy ($E_F=0$ in fig. 2) at $\omega=0$. The corresponding non-interacting levels are shown in fig. 3, where they are labelled 1, 2, 3, ... and -1, -2, -3, ... respectively. The levels filled in the yrast-configuration are drawn as thick lines. We see immediately that the yrast configuration changes its character at the frequencies ω_1 and ω_3 . For the interpretation of some other low-lying configurations we refer to table 1.

3. PARAMETER VALUES AND THE SELF-CONSISTENCY CONDITION

Equation (2.1) contains three adjustable parameters, viz. the Fermi energy, λ , the rotational frequency, ω , and the pairing gap, Δ . In this paper the Fermi energy is determined by the constraint that the expectation value of the particle number, $\langle N \rangle$, should be six. The results which we are going to discuss are not strongly dependent on the value chosen for the particle number, and the restriction to one particle number is not a serious limitation of the generality of the conclusions. On the other hand we shall treat ω and Δ as independent variables and discuss the solutions of the HFB-equations as functions of these variables.

Depending on the configuration and the frequency there may exist one or more self-consistent (non-zero) values of the gap, defined by the condition

$$\Delta_{\text{s.c.}} = G \sum_{m,n} P_{mn} \tau_{nm}, \quad (3.1)$$

where P_{mn} are the matrix elements of the operator $(a_m^+ a_{\bar{m}}^+ + a_{\bar{m}} a_m)$ and τ_{mn} those of the pairing tensor.

One may also consider the energy in the rotating frame of reference

$$E' = \sum_{\alpha, m, n} (\epsilon_{mn}^{\alpha} - \omega (j_x)_{mn}^{\alpha}) \rho_{nm}^{\alpha} - G (\sum_{mn} P_{mn} \tau_{nm})^2 + \lambda \langle N \rangle, \quad (3.2)$$

where $\langle N \rangle = \sum_{\alpha, m, n} \rho_{nm}^{\alpha}$ and ρ_{nm}^{α} are the matrix elements of the density matrices (one for each signature, α). The energy matrix elements $\epsilon_{mn}^{\alpha} = e_{mn} - \lambda \delta_{mn}$ are in our case diagonal, cf. eq. (2.2). If the energy, E' , is considered as a function of Δ for fixed value of ω , the self-consistent solutions are given by the condition $\partial E' / \partial \Delta = 0$. As will be seen later this may correspond either to a maximum or a minimum of E' as a function of Δ . The value of $\Delta_{\text{s.c.}}$ is strongly dependent on the value of G . In this work we use $G = 0.125 \text{ MeV} \approx 0.32 \text{ K}$, which is relatively large compared to the value 0.206 K used in refs. (12,13). The corresponding value of $\Delta_{\text{s.c.}}$ therefore becomes large, for the ground configuration roughly three times the experimental value.

The large value of G can, however, be justified for the following reasons. We want to study a situation where the self-consistent pairing gap of

the lowest 2 q.p.-configuration (s-configuration) is non-zero, since this seems to be the actual physical situation (cf. fig. 1). It is furthermore desirable that $\Delta_{s.c.} \gtrsim 0.1 \hbar\omega_0$ for the s-configuration, since for small values of Δ the wave function of this configuration undergoes sudden and dramatic changes (see table III), as a result of the variation in λ that is necessary for fulfilling the constraint $\langle N \rangle = 6$. This is quite a general property of excited configurations, appearing when Δ becomes small enough compared to the average level splitting. In more realistic calculations, including also the negative parity levels, the average level splitting is much smaller. This has a stabilizing effect and the wave functions change in a smooth way well below the Δ -values of physical interest (cf. fig. 1). We have therefore found the above choice of G to be optimal in order to obtain such solutions as, within our limited space, reproduce as closely as possible the main structures of the solutions obtained in full scale calculations.

4. CALCULATION OF SELF-CONSISTENT SOLUTIONS USING THE NON-INTERACTING LEVELS

The quasiparticle levels shown in fig. 2 are representative for the $i_{13/2^-}$ shell (or any other high-j shell) in what concerns the appearance of certain easily recognizable pseudo level crossings, like those indicated by the arrows. The general pattern remains essentially the same, when the Fermi energy moves from the bottom up towards the top of the shell. Also as a function of Δ the level structure shows an amazing stability, except for very small values of Δ , where in the limit $\Delta=0$ we can no longer distinguish the characteristic pseudo crossings. The reason is that the interaction between the levels involved in the pseudo crossings increases strongly when Δ approaches zero, so that finally near-lying pseudo crossings merge together and can no longer be identified.

In the limit $\Delta=0$ the quasiparticle levels become identical to the single-particle levels, except for a duplication of the levels due to a reflexion in the Fermi surface, see ref. ¹¹⁾. As is seen from fig. 4, the single-particle level diagram looks very different from the corresponding quasiparticle level diagram in fig. 2. (One may imagine a reflexion in the Fermi surface to make the comparison adequate.) In particular we do not find the typical pseudo crossings, and as a

consequence, it is no longer possible to define a set of non-interacting levels as in section 2 (cf. fig. 3).

In practice the construction of the non-interacting levels is hardly possible for $\Delta \lesssim 0.05 \hbar\omega_0$ (≈ 0.4 MeV). Therefore they cannot serve as a tool for studying the last stages in the transition from the superfluid to the normal phase (breakdown of pairing due to the Coriolis-anti-pairing effect, cf. section 9). However, for investigating bandcrossings, where the essential change is the alignment of individual quasiparticles, the introduction of the non-interacting levels leads to a great simplification and might be indispensable at high rotational frequencies, where the pseudo crossings appear with short intervals.

When one eliminates the interaction at the pseudo crossings it is most convenient to keep Δ and λ fixed, and therefore the following procedure has been used to find the self-consistent solutions. For a number of grid-points (Δ, λ) , the quasiparticle levels are calculated as functions of ω , and the interactions are eliminated. Normally one is only interested in eliminating a few of the first interactions, in particular those marked in fig. 2. The resulting non-interacting quasiparticle energies and wave functions are stored, since they can be used later for investigating excited configurations. At each point $(\Delta, \lambda, \omega)$, we calculate the needed expectation values e.g. $\langle N \rangle$, $\langle J_x \rangle$, etc. By interpolation in λ , we find those values of these quantities, which correspond to the desired particle number, N , and we calculate the energy $E' = E'_N(\Delta, \omega)$ (see eq. (3.2)). For fixed values of ω we then use an interpolation procedure to determine at which value of Δ the energy E' has its minimum (note that we do not get multiple solutions when we use the non-interacting levels). This gives us the self-consistent solutions $E'_N(\Delta_{s.c.}, \omega)$, which may be displayed as a function of ω . The corresponding values of other quantities, such as $\langle J_x \rangle$, are obtained by interpolation between the grid-points in Δ .

In fig. 5 we show the values of $\Delta_{s.c.}$ (solid lines) obtained for the g- and the s-configurations, keeping $\langle N \rangle = 6$. The frequencies of the pseudo crossings are shown by the dot-dashed lines. Notice that the crossing frequencies increase with Δ , and that the crossings at ω_2^I and ω_2^{II} only affect the g-configuration, cf. table I. As expected, $\Delta_{s.c.}$ goes through the crossing frequencies without showing any irregularities. In fact it turns out that $\Delta_{s.c.}$ is practically independent of ω . This is quite

natural, since the non-interacting levels form more or less straight lines, indicating that the quasiparticle wave functions are almost independent of ω . This can also be illustrated by calculating the overlap between the many-body wave functions corresponding to different frequencies. Thus for the g-configuration we obtain an overlap of 0.95 between the wave functions calculated at $\omega/\omega_0 = 0.03$ and 0.075. For the s-configuration the corresponding value is 0.82. This clearly shows that the non-interacting configurations indeed conserve their character through the crossings.

In a realistic case, where all relevant levels in the vicinity of the Fermi surface are included, the situation is slightly different, since the quasiparticle levels which do not belong to the high-j shell (we shall here call them the core levels) gradually build up a collective angular momentum as ω increases. The overlap integrals between the total many-body wave functions given above will then become small or even vanish, depending on how profoundly the core has changed its character. However, since all well-developed pseudo crossings appear only in the high-j shell ¹¹⁾, the total many-body wave function, constructed from the non-interacting high-j levels plus the core levels, will change its structure smoothly due to small changes in a large number of individual quasiparticle wave functions. When ω increases, one cannot distinguish any frequency where the change is considerably faster than on the average and we get a regular unperturbed rotational band. One should not expect, however, that $\Delta_{s.c.}$ remains more or less constant within a given configuration. The gradual increase of the core angular momentum will in fact lead to a smooth reduction of $\Delta_{s.c.}$. This can be seen e.g. in ref. ¹⁵⁾ if one disregards the perturbations in the backbending regions.

The technique described above for eliminating the interactions remains feasible in a realistic calculation since those pseudo crossings which have to be eliminated appear only in the high-j shell, and therefore the computational effort for eliminating them does not increase compared to our $i_{13/2}$ model. Furthermore, the number of gridpoints (Δ, λ) can be kept small, because once the interactions are eliminated all variables become smooth well-behaved functions. Therefore the calculational technique described in this section can be used in realistic calculations without increase in computer time, compared to what is normal in this kind of work.

5. PARTICLE NUMBER PROJECTION

The linearized HFB-Hamiltonian of eq. (2.1) does not commute with the particle number operator. Consequently it generates wave functions which do not have well-defined particle number. Therefore it has long been customary to perform particle number projection¹⁷⁾, thus hopefully creating a better approximation to the eigenstates of the exact Hamiltonian, which in our case reads

$$H = \sum_m (e_m - \lambda) a_m^\dagger a_m - \omega \sum_{m,n} \langle m | j_x | n \rangle a_m^\dagger a_n - G \sum_m a_m^\dagger a_m^\dagger \sum_n a_n a_n \quad (5.1)$$

The energy of the particle-number-projected wave function is then calculated as the expectation value of this Hamiltonian.

As stated in the Bloch-Messiah theorem¹⁸⁾ there always exists a single particle basis, the so called canonical basis, that brings the density matrix and the pairing tensor on a diagonal form simultaneously. (For details, see e.g. the work by Goodman¹⁹⁾.) The use of this basis facilitates the projection considerably, because the HFB wave function, $|HFB\rangle$, then takes the congenial BCS-form

$$|HFB\rangle = \prod_v (u_v + v_v a_v^\dagger a_v^\dagger) |-\rangle. \quad (5.2)$$

It should be observed that the conjugate states $a_v^\dagger |-\rangle$ and $a_{\bar{v}}^\dagger |-\rangle$ in general do not correspond to a pair of time-reversed states. In fact, for $\omega \neq 0$ they may have very little resemblance of such a pair although they have the same occupation probability, i.e. $|v_v| = |v_{\bar{v}}|$. However, the formalistic advantages of the BCS-wave function remain, which we have exploited for the particle number projection. By making a simple expansion of the product wave function, (5.2), we get

$$|HFB\rangle = \left\{ \prod_{k=1}^{c/2} u_k + \prod_{k=1}^{c/2} u_k \sum_{i=1}^{c/2} \prod_{j=1}^i \left(\sum_{k_j=1}^{c/2} \frac{v_{k_j}}{u_{k_j}} a_{k_j}^\dagger a_{\bar{k}_j}^\dagger \right) \right\} |-\rangle \quad (5.3)$$

where $k_j < k_{j+1}$ and c is the number of accessible single-particle states. Using the u 's and the v 's of the HFB-solutions we can immediately extract from (5.3) that wave function, which corresponds to the desired particle number. In cases where the dimension of the single-particle basis and the number of active particles are much larger than here, this method becomes too time-consuming. Nevertheless, in our case the calculation time is negligible, and the fact that we get exact information about the

projected wave function makes the projection technique outlined above more adequate for our purpose than other existing projection methods.

6. APPLICATION OF THE PARTICLE NUMBER PROJECTION TO THE NON-INTERACTING QUASIPARTICLE CONFIGURATIONS

The easiest way to obtain particle number projected solutions would be to make a projection from the final states, $E_N^i(\Delta_{s.c.}, \omega)$ of section 4 ("projection after minimization"). On the other hand, it is not clear that the value found for $\Delta_{s.c.}$ before projection remains the optimal one, i.e. corresponds to the lowest energy, after projection. An alternative procedure would therefore be to make a projection at each point, (Δ, ω) , using the non-interacting wave functions, and then minimize the energy with respect to Δ , using the same interpolation technique as outlined in section 4 ("minimization after projection").

The constraint $\langle \hat{N} \rangle = N$ has no meaning after projection, since it is trivially fulfilled. One could therefore in principle also allow λ to vary when searching for the optimal particle number projected solution. For the yrast configuration there are hardly any objections against such a procedure, which we have tested in a couple of cases. It was then found that the optimal λ might be quite different from the one, λ_N , giving $\langle \hat{N} \rangle = N$. However, the projected wave function showed a great insensitivity to the variation in λ , and the optimal solution was practically identical to the one calculated at $\lambda = \lambda_N$. For excited configurations such a variation of λ may be more doubtful, cf. section 7. The particle number projected results presented in this paper are therefore those obtained after minimization of the projected energies with respect to Δ , under the constraint that $\langle \hat{N} \rangle = N = 6$ for the unprojected wave functions.

In fig. 5 we show the values of $\Delta_{s.c.}$ obtained after particle number projection to $N=6$ (the dashed lines). For the g-configuration $\Delta_{s.c.}$ is almost equal to what was obtained without projection, except for an overall increase of about 10%. For the s-configuration the increase is much more pronounced ($\approx 60\%$). We also observe that when we approach $\omega=0$ the selfconsistent gap calculated before projection decreases, while the gap calculated after projection increases. This is connected with the relatively complicated behaviour of the s-configuration wave function at small frequencies. In fact, for $\omega=0$, the s-configuration cannot be defined

under the constraint $\langle \hat{N} \rangle = 6$ (or any other even particle number), since independently of Δ the expectation value $\langle \hat{N} \rangle$ makes a discontinuous jump each time the Fermi energy lies exactly between two single-particle levels. It is only when the single-particle levels split up due to the rotation (cf. fig. 4) that $\langle \hat{N} \rangle$ can reach an even integer number. This can easily be understood by looking on how $\langle \hat{N} \rangle$ is calculated from the density matrix.

For $\omega/\omega_0 = 0.02$ we have made calculations also for some other low-lying configurations. In all cases we observe an increase of $\Delta_{s.c.}$ after projection. This is not a peculiarity of the $i_{13/2}$ -model, but has been observed also in other calculations²⁰⁾.

7. COMPARISON BETWEEN PARTICLE NUMBER PROJECTED AND NON-PROJECTED SOLUTIONS

In order to understand the effect of particle number projection, one has to know the distribution over different particle numbers in the unprojected wave function. This is shown in the lower part of fig. 6 for $\omega/\omega_0 = 0.01$. The ground configuration starts with exactly 6 particles at $\Delta=0$. With increasing Δ -values, the probability for 6 particles decreases rapidly until Δ reaches $0.2 \hbar\omega_0$, where it is already smaller than 0.5, while for larger Δ -values it levels out. Instead the probability for having 4 or 8, but also 2 or 10, particles increases. For the s-configuration the situation is similar if one neglects what happens for $\Delta \leq 0.1 \hbar\omega_0$. We shall, however, come back to this point later.

7.1 The increase of the selfconsistent pairing gap due to projection

Having the projected wave functions, the energies corresponding to the various particle numbers may be calculated as the expectation value of the Hamiltonian (5.1). They are shown in the upper part of fig. 6 by the solid lines, marked with the corresponding particle numbers. The unprojected energy, denoted H , is given by eq. (3.2). It must, however, be observed that the Hamiltonians (2.1) and (5.1) do not give the same energy even for a wave function calculated with $\Delta=0$, and thus having well-defined particle number, since the term $G \sum_m a_m^+ a_m^+ \sum_n a_n^- a_n^-$ will give

a contribution to the energy also in this case. We have therefore displaced the unprojected energies (H) downwards (≈ 3 G for the g-configuration and ≈ 2 G for the s-configuration), so that they start at the same energy as the corresponding six-particle curves at $\Delta=0$.

The occupation-number-weighted average (E_a) of the projected energies is also shown in fig. 6 (curve a). It is approximately related to the unprojected energy (H) through

$$E_a \approx E_H - G \sum_i v_i^4 P_{ii}^2, \quad (7.1)$$

where v_i^2 is the occupation probability of the canonical basis state $|i\rangle$ and P_{ii} is the corresponding diagonal matrix element of $(P^\dagger + P)$ in the canonical basis. The term $-G \sum_i v_i^4 P_{ii}^2$ accounts for the difference between the Hamiltonians (2.1) and (5.1). For small values of Δ this term is $\approx 3G$ for the g-configuration and $\approx 2G$ for the s-configuration (in fig. 6 the H-curves have been lowered by these quantities).

In fig. 6 we have chosen the constant e_0 of eq. (2.2) equal to $0.2 \hbar\omega_0$. The value of e_0 does not change the relative position of the curves marked a, H and 6 since they all have $\langle N \rangle = 6$. However, the relative position of the curves corresponding to different particle numbers is dependent on e_0 . The above choice of e_0 facilitates the subsequent discussion since it gives the lowest energy to the projected $N=6$ state. The conclusions are, however, independent on the value of e_0 .

We can now easily understand those properties of the g-configuration which result from the non-conservation of the particle number. With increasing Δ the content of $N=6$ falls off rapidly, and the fractions of $N = 2, 4, 8, 10$, gradually increase. Since these particle numbers correspond to higher energies, the average energy (a), soon becomes considerably higher than the $N=6$ energy. For small values of Δ , where the $N=6$ component is still dominating, the average energy decreases, but quite soon the increasing admixture of other particle numbers makes the average energy increase. In fact, the average energy has its minimum at a lower Δ -value than any of the individual particle-number-projected energies. The relation between the unprojected energy E_H and the projected energies is slightly more complicated because the term $G \sum_i v_i^4 P_{ii}^2$ appearing in eq. (7.1) is not independent of Δ , but

decreases slowly. Therefore the unprojected energy follows the projected $N=6$ energy closer than the average energy does, although qualitatively nothing is changed.

For the s-configuration the situation is essentially the same if one neglects what happens for $\Delta \leq 0.1 \hbar\omega_0$. The displacement of the energy minimum due to projection is larger, however, mainly because the unprojected minimum lies at $\Delta = 0.13 \hbar\omega_0$, a point at which the $N=6$ component is still decreasing relatively fast and consequently the energy gain due to projection increases markedly with Δ . For larger values of Δ , where the distribution on different particle numbers changes only slowly the curves marked a, H and 6 become practically parallel, and the displacement of the energy minimum after projection is relatively small as in the g-configuration. This explains why the difference in $\Delta_{s.c.}$ between the s- and g-configurations becomes considerably reduced after particle number projection.

It is thus the increasing impurity in particle number and the accompanying increase in energy that pushes the minimum in the unprojected energy towards a smaller value of Δ than is found for the particle number projected energy. This is a general feature found in all cases which we have investigated.

7.2 Non-orthogonality between the particle-number-projected configurations

Not even the unprojected wave functions are completely orthogonal, since $\Delta_{s.c.}$ is not the same for all configurations. The desired particle number is rarely contained to more than 50% in the unprojected wave function and as a consequence the particle number projected wave functions may show a considerable overlap.

The non-orthogonality between the particle number projected configurations is further accentuated by the fact that the number of quasiparticle configurations is larger than the number of single-particle configurations. With 6 particles in the $i_{13/2}$ shell one obtains in total 3003 orthogonal single-particle configurations. The number of quasiparticle configurations with integer signature, and thus corresponding to even particle numbers, is 8192. All of these can in principle for $\Delta \neq 0$ contain a certain fraction

of $N=6$ components, and therefore the particle number projected wave functions cannot in principle all be orthogonal. Another consequence is that one cannot generally say that a given quasiparticle configuration corresponds to a certain single-particle configuration. This has to be kept in mind when one studies the break-down of pairing (cf. section 9). Even if $\Delta_{s.c.}$ apparently may go smoothly to zero, the wave function can undergo drastic changes, and it may in the limit $\Delta_{s.c.}=0$ have no particular similarity to that of the quasiparticle configuration that preceded it.

One may approach the limit $\Delta=0$ in two ways and with somewhat different results. If λ is kept fixed, the quasiparticle configurations go over into single-particle configurations with different particle numbers. This is because the number of quasiparticle configurations is equal to the total number of single-particle configurations of even particle number. If on the other hand the particle number $\langle N \rangle$ is kept fixed, several quasiparticle configurations go over into the same single-particle configuration. It is, however, not always possible to obtain all values $\langle N \rangle$ for a given quasiparticle configuration, cf. section 6.

7.3 Characteristic labels of the particle number projected wave functions

The lack of orthogonality between the particle number projected wave functions may cast some doubt on how good approximations they are to the eigenstates of H of eq. (5.1). However, for the low-lying configurations the overlap is normally reasonably small (cf. ref. ²²⁾). Thus the overlap between the self-consistent g- and s-configurations is smaller than 0.08 for $\omega/\omega_0 > 0.02$ while for smaller frequencies it takes somewhat higher values. We therefore believe that the low-lying particle-number-projected states in general are good approximations, not only to the eigenstates of the Hamiltonian (5.1) but also to the observed physical states. This assumption is further supported by the fact that the quasiparticle levels themselves can be closely related to the experimental excitation energies of various configurations ¹¹⁾. Consequently one has to conclude that the lowest excited configurations that can be constructed from the quasiparticle levels can be given

distinct labels which separate them from each other and make it possible to identify them uniquely with the observed rotational bands, at least if λ is chosen such that $\langle N \rangle$ is approximately equal to the correct particle number. The label of a configuration is the appearance of certain components in the wave function. These components can be directly associated with the specific excitations made for constructing it (see subsection 7.4). Normally this label survives the particle number projection and is easily recognizable in the projected wave function. Varying Δ within reasonable limits does not change the specific label of the configuration, although the overall degree of excitations to higher-lying single-particle states is considerably changed (cf. table III). A minimization of the energy with respect to Δ then corresponds to an optimization within a space which is intimately connected with the given excited configuration. Whether this space is sufficiently large and the label sufficiently distinct depends in its details on the mutual relation between the Hamiltonians of eqs. (2.1) and (5.1) and on their ability to generate approximations to the observed states.

The configuration labels are often sensitive to the position of the Fermi surface. In order to ensure a well-defined label it is therefore important to choose λ so that the correct particle number is reproduced, since we know that for this value of λ the agreement between the quasi-particle levels and the experimental excitation energies is optimal.

7.4 Properties of the s-configuration for small values of Δ

The particle number projected energies of the s-configuration show dramatic changes for $\Delta \leq 0.15 \hbar\omega_0$ (see fig. 6), although the unprojected energy (H) behaves smoothly. The reason for this can be traced back to an important rearrangement that takes place in the wave function when Δ becomes smaller than the single-particle level splitting at the Fermi surface, which in our case is $0.144 \hbar\omega_0$ (between the $m=5/2$ and $7/2$ levels). The behaviour of the s-configuration is representative for excited configurations and is closely connected with the sometimes quite delicate adjustment of λ that is necessary in order to keep the particle number fixed when Δ is smaller than the average level splitting at the Fermi surface.

In fig. 6, where $N=6$, we see that of all the projected energies it is the $N=6$ component that shows the most regular behaviour. Its wave

function is shown in table III for some values of Δ . The characteristic label of the s-configuration for $N=6$ are the components $\alpha | \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{7}{2}, \frac{3}{2}, \frac{1}{2} \rangle + \beta | \frac{7}{2}, \frac{3}{2}, \frac{1}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle$ with $\alpha \approx \beta$. These terms describe an excitation of a particle from the $m=5/2$ to the $m=7/2$ single-particle level in which the excitation probability is equal for the two signatures. The wave function also contains a less important term $\gamma | \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{7}{2}, \frac{5}{2}, \frac{1}{2} \rangle + \delta | \frac{7}{2}, \frac{5}{2}, \frac{1}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle$ ($\gamma \approx \delta$) which is characteristic and might be included in the label. It describes an excitation from the $m=3/2$ to the $m=7/2$ single-particle levels. The other terms are of the same kind as those appearing in the g-configuration: $|m_1, m_2, m_3, \bar{m}_1, \bar{m}_2, \bar{m}_3\rangle$, and are not specific for the s-configuration.

The label components dominate the s-configuration except for $\Delta=0$, where $| \frac{7}{2}, \frac{3}{2}, \frac{1}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle$ disappears and $| \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{7}{2}, \frac{3}{2}, \frac{1}{2} \rangle$ practically takes over all the strength. Although it is possible to follow the s-configuration, defined as the lowest 2 quasiparticle excitation, to the limit $\Delta=0$ as in fig. 6, we must not forget that its structure changes completely. (This is, however, not the case for all frequencies as will be discussed in section 9.) At $\Delta=0$ the s-configuration becomes a 1p1h single-particle configuration. There exists, however, no 1p1h configuration at $\omega/\omega_0=0.01$ which contains the typical label of the s-configuration. This label can only be constructed as a linear combination of two different 1p1h configurations. The 1p1h configuration reached in the limit $\Delta=0$ corresponds to exciting one particle from the level C to the level D in fig. 4.

For the other particle number projected wave functions the changes with Δ are more pronounced, and quite similar for the different particle numbers. Thus for $\Delta=0.25 \hbar\omega_0$ the $N=8$ wave function is

$$\begin{aligned} & 0.4277 | \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle + 0.3544 | \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle + \\ & 0.3019 | \frac{9}{2}, \frac{7}{2}, \frac{3}{2}, \frac{1}{2}, \frac{9}{2}, \frac{7}{2}, \frac{3}{2}, \frac{1}{2} \rangle + 0.3207 | \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{9}{2}, \frac{7}{2}, \frac{3}{2}, \frac{1}{2} \rangle + \\ & 0.3238 | \frac{9}{2}, \frac{7}{2}, \frac{3}{2}, \frac{1}{2}, \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle + 0.2063 | \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle + \\ & 0.2067 | \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle + \dots \end{aligned}$$

We notice that the label $\alpha | \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle + \beta | \frac{9}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2} \rangle$, which is the dominating and characteristic component in the $N=8$ s-configuration determined under the condition $\langle N \rangle = 8$ appears here with a relatively small

amplitude. This illustrates the statement in section 7.3, saying that the typical table is lost if $\langle N \rangle$ is too far away from the desired particle number.

When Δ decreases below $\approx 0.15 \hbar\omega_0$ the wave function undergoes large rearrangement, and for $\Delta=0.05 \hbar\omega_0$ it is

$$0.9784 \left| \begin{smallmatrix} 7 & 5 & 3 & 1 & \bar{7} & \bar{5} & \bar{3} & \bar{1} \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{smallmatrix} \right\rangle + 0.1425 \left| \begin{smallmatrix} 7 & 5 & 3 & 1 & \bar{9} & \bar{5} & \bar{3} & \bar{1} \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{smallmatrix} \right\rangle + \\ 0.1426 \left| \begin{smallmatrix} 9 & 5 & 3 & 1 & \bar{7} & \bar{5} & \bar{3} & \bar{1} \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{smallmatrix} \right\rangle + \dots$$

A further decrease of Δ hardly changes the wave function. We see that even if the label components still appear, the wave function is to 96% $\left| \begin{smallmatrix} 7 & 5 & 3 & 1 & \bar{7} & \bar{5} & \bar{3} & \bar{1} \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \end{smallmatrix} \right\rangle$, i.e. the $N=8$ s-configuration wave function is practically identical to the corresponding single-particle g-configuration (at $\omega/\omega_0=0.01$), and does not at all describe an excited configuration. The situation is similar for $N=2,4$ and 10 . The minimal energies, obtained for $\Delta \approx 0.05 \hbar\omega_0$, are also very close to those which can be calculated from the single-particle levels of fig. 4 by filling the corresponding number of particles into the lowest levels. (One has to take into account that different values for e_0 have been used in figs. 4 and 6 and that one must include the term $-G \sum_i v_i^4 P_{ii}^2$.)

Below $\Delta \approx 0.10 \hbar\omega_0$ the probability for 6 particles decreases while those for 4 and 8 particles increases. This can be understood if one considers what happens for $\omega/\omega_0=0$, where levels with the same m have the same energy. The expectation value of the number operator, $\langle N \rangle$, then has a discontinuity at the λ -value right between the $m=5/2$ and $m=7/2$ levels. At this λ -value $\langle N \rangle$ jumps from ≈ 4 to ≈ 8 . These particle numbers are also dominating the corresponding wave functions, especially for small values of Δ . At $\omega/\omega_0=0.01$ the situation is different, since the $m=5/2$ and $m=7/2$ levels both show a signature splitting, which, although very small ($0.0005 \hbar\omega_0$ for $m=5/2$) allows $\langle N \rangle$ to increase continuously from ≈ 4 to ≈ 8 in a very narrow interval of λ . It may thus take the value 6, although at this point the wave function is to 50% a mixture of $N=4$ and $N=8$. The $N \neq 6$ component do not decrease to zero until Δ becomes smaller than the signature splitting. In this limit the $N=6$ component (with probability 1) goes over into the $1p1h$ configuration discussed above.

The discussion above shows that one has to be extremely careful when treating excited configurations, and that one always has to make sure that the (self-consistent) solution found really has the characteristic properties (label) of the experimental state that it is supposed to describe.

8. BANDCROSSINGS AT HIGHER FREQUENCIES

In some recent publications the solutions of the (self-consistent) cranked HFB-model have been discussed in detail ^{4,23)}. Especially the unphysical behaviour of the solutions near the bandcrossings (i.e. the pseudo crossings in the quasiparticle diagrams) has been carefully investigated. As concluded by Marshalek and Goodman ⁴⁾ but also pointed out earlier by Hamamoto ¹²⁾ there is no way of overcoming these difficulties if one applies the HFB-model literally.

In a couple of papers ^{9,15)} the spurious solutions near the bandcrossings have been omitted and the complete g- and s-bands have been constructed by interpolating between the well-behaved parts of these bands before and after the pseudo crossing, roughly corresponding to the use of the non-interacting levels (fig. 3). In cases of weak interactions this seems to be a straightforward method yielding results in good agreement with experiment.

At higher frequencies the situation is further complicated by the fact that the pseudo crossings become more and more frequent (cf. table I and figs. 2-3), so that the frequency intervals in which non-spurious solutions can be found are strongly reduced. To illustrate the nature of the problems which arise, we have in fig. 7 plotted $E_N^i(\Delta, \omega)$ for the vacuum configuration, which has a relatively simple behaviour, as it changes character only at ω_1 and ω_3 (cf. table I). To the left of ω_1 we recognize the energy surface corresponding to the g-configuration, between ω_1 and ω_3 that of the s-configuration and to the right of ω_3 that of the 3rd configuration. Near the dashed lines, indicating the interaction frequencies, the surfaces go over into each other. This gives rise to a more or less complicated structure, which is particularly pronounced at ω_1 while at ω_3 it appears only as a slight change in the slope of the energy lines.

The Δ -values corresponding to the self-consistent solutions (eq. (3.1)) are shown by the dot-dashed line, which also corresponds to $\frac{\partial E_N(\Delta, \omega)}{\partial \Delta} = 0$. For the non-spurious solutions this gives a minimum in $E_N(\Delta, \omega)$ if it is considered as a function of Δ for fixed value of ω . However, for the backgoing part, following ω_1 , which is responsible for the unphysical solutions it gives a maximum.

The quasiparticle energy diagrams give, in fact, the key for understanding fig. 7, since they not only define the crossing frequencies, but also give the interaction strength. Taking the results obtained for the non-interacting levels as a reference, the interpretation becomes transparent. To the left of ω_1 the energy surface corresponds to that of the g-configuration. Consequently the self-consistent gap lies around $0.34 \hbar\omega_0$ (cf. fig. 5). At this value of Δ the interaction at ω_1 is considerably weaker than at $\Delta=0.15 \hbar\omega_0$ shown in fig. 2, and therefore $\Delta_{s.c.}$ stays equal to that of the non-interacting g-configuration almost up to ω_1 . Above ω_1 the vacuum takes the character of the s-configuration, for which $\Delta_{s.c.}$ is much smaller ($\approx 0.15 \hbar\omega_0$, cf. fig. 5). For this value of Δ the crossing frequency is considerably reduced, and therefore the self-consistent solution follows closely (due to the small interaction) ω_1 backwards to smaller frequencies until a value of $\Delta_{s.c.}$ corresponding to that of the s-configuration is reached. If no further crossings had occurred $\Delta_{s.c.}$ would have been stabilized close to this value like in fig. 5. However, at ω_3 the vacuum configuration meets a new pseudo crossing. The interaction is here relatively stronger than at ω_1 (mainly due to the decrease in Δ) and therefore the vacuum configuration is affected by this crossing well before ω_3 . In fact it has just established the character of the s-configuration before it starts to feel the interaction and $\Delta_{s.c.}$ goes to zero, which is the self-consistent solution to the 3rd configuration. Because of the strong interaction the frequency ω_3 is never approached closely and we do not get any backbending.

In fig. 8 $\Delta_{s.c.}$ is shown also for some other configurations. The figs. 2 and 3 and the tables I and II contain the necessary information for understanding the behaviour of $\Delta_{s.c.}$. Thus the configuration [a,b,-c,-d] starts as the s-configuration. At ω_1 it goes over into the g-configuration and when ω approaches ω_2' , a strong backbending is produced, which, however, is stopped at $\Delta_{s.c.} \approx 0.12 \hbar\omega_0$, corresponding to the self-consistent gap of the 4th configuration. Then follows a dip down to $\Delta=0$ as [a,b,-c,-d] goes over into the 3rd configuration, while finally the

character of the s-configuration is reestablished when passing the pseudo crossing at ω_3 . We have also shown the configurations which successively build up the g-configuration between the various pseudo crossings. The meaning of the non-interacting g-configuration (the upper dotted line) becomes clear in this picture as a smooth interpolation across the interaction frequencies. Also for the s-configuration one may imagine how it is built up successively by the configurations $[a,b,-c,-d]$ (for $\omega < \omega_1$), the vacuum (for $\omega_1 < \omega < \omega_3$) and once again $[a,b,-c,-d]$ (for $\omega > \omega_3$). The large interactions at the low Δ -values appropriate for the s-configuration make the situation less clear. Especially the strong interaction at ω_3 which causes the gap of the vacuum to collapse very early when ω approaches ω_3 , and that of $[a,b,-c,-d]$ to increase slowly, makes it in this case impossible to construct the continuation of the s-configuration (the lower dotted line) directly from the interaction quasiparticle levels. It should be observed that the interaction strength is strongly dependent on λ ²⁴⁾. For other values of λ which do not correspond to an even integer number of particles ²⁵⁾ in the $i_{13/2}$ shell, the interaction becomes smaller or even vanishes. In such cases the continuation of the s-configuration can be obtained in a simple way from the interacting solutions.

If the non-interacting solutions are used for calculating rotational bands one obtains a number of sharply crossing bands like in fig. 9, showing the first 3 bands building up the yrast line. At each crossing a more or less sharp backbending is produced. The non-interacting configurations are therefore only suitable for describing band crossings with small or vanishing interaction, i.e. they should be used in cases where the literal application of the HFB-model gives its worst results. The non-interacting configurations may, however, be used also in cases where the interaction is not negligible, namely if an interaction is introduced between the rotational bands, acting between states with the same angular momentum (in practice the same value of $\langle J_x \rangle$). This possibility has been considered by Hamamoto ¹²⁾. However, for more realistic applications a more detailed understanding of the true nature of the interaction would be highly desirable.

If a reasonable manybody Hamiltonian is known a more satisfactory approximation to the real rotational states can be obtained by a simple diagonalization in a basis of two orthogonalized states obtained from the g- and the s-configurations. This technique allows us to include other low-

lying states than those belonging to the two interacting configurations. However, even if particle number projected states are used, the final states will suffer from a severe deficiency concerning the angular momentum. As shown in ref. ¹⁰⁾ the HFB-states show a very large spread in angular momentum, and a considerable improvement can be expected if one could perform angular momentum projection. Starting from the particle number projected states the technique described in ref. ¹⁴⁾ is in principle directly applicable. In practice, however, it can only be used for light nuclei with a small number of particles outside closed shells. It would therefore be highly desirable to develop a projection technique which, with a reasonable computational effort, can be applied to e.g. nuclei in the rare earth region (cf. ref. ²⁾) and to investigate whether a small configuration space, spanned by particle-number and angular-momentum projected states obtained from the lowlying HFB-configurations, is sufficient for describing the rotational states near the yrast line.

9. BREAK DOWN OF PAIRING

The non-interacting configurations give essential information about changes of the pairing properties with increasing rotational frequency. Within a given configuration it is only the Coriolis antipairing effect that can change the pair correlations and eventually lead to a transition to the normal phase. Rotational alignment of individual pairs of quasi-particles is excluded, because it would by definition correspond to a transition to another non-interacting configuration.

Although the non-interacting configurations cannot be constructed for $\Delta \leq 0.05 \hbar \omega_0$, they are very useful for understanding also the last stages in the breakdown of pairing. Thus we can immediately conclude that the disappearance of pairing at $\omega/\omega_0 \approx 0.048$ in the vacuum configuration, shown in fig. 7, is caused by rotational alignment of a second pair of quasi-particles, which changes the character of the vacuum from that of the s-configuration to that of the 3rd configuration. We can exclude that the breakdown is due to the Coriolis antipairing effect within the s-configuration, because for the non-interacting s-configuration the pair correlations remain up to much higher rotational frequencies (see fig. 5). That this conclusion is correct can also be understood from fig. 10,

showing the overlap between the unpaired vacuum $[A,B,C,\bar{A},\bar{B},\bar{C}]$ (with the labels of fig. 4) and the three particle number projected quasiparticle configurations g, s and 3 (with $\Delta=0.15 \hbar\omega_0$).

At $\omega/\omega_0=0$ the wave function of the unpaired vacuum $[A,B,C,\bar{A},\bar{B},\bar{C}]$ is $|\frac{5}{2},\frac{3}{2},\frac{1}{2},\frac{5}{2},\frac{3}{2},\frac{1}{2}\rangle$ which to 86% overlaps with that of the g-configuration (cf. table III). With increasing frequency the low-lying levels of fig. 4 align gradually and at $\omega/\omega_0\approx 0.035$ the dominating component in $[A,B,C,\bar{A},\bar{B},\bar{C}]$ is $\alpha|\frac{5}{2},\frac{3}{2},\frac{1}{2},\frac{7}{2},\frac{3}{2},\frac{1}{2}\rangle + \beta|\frac{7}{2},\frac{3}{2},\frac{1}{2},\frac{5}{2},\frac{3}{2},\frac{1}{2}\rangle$, which is the characteristic label of the s-configuration. This is reflected in an overlap with the s-configuration of more than 90%. At still higher frequencies ($\omega/\omega_0\geq 0.05$) all the six lowest levels of fig. 4 are approaching their final alignment, and the wave function of $[A,B,C,\bar{A},\bar{B},\bar{C}]$ becomes more and more close to that of the 3rd configuration. For this configuration the only self-consistent solution has $\Delta=0$, and it coincides at sufficiently high frequencies with the unpaired vacuum. This is clearly seen in fig. 10 where the overlap between the 3rd configuration and the unpaired vacuum approaches 100%.

As clearly pointed out in section 4 we see in the $i_{13/2}$ model very small structural changes in a non-interacting configuration even if we go to very high frequencies. The breakdown of pairing along the yrast line therefore gets a very simple explanation as being caused by a successive alignment of pairs of quasiparticles: No aligned pair in the g-configuration, one pair in the s-configuration and two pairs in the 3rd configuration. The configuration changes along the yrast line are shown in fig. 9 where we also show the unpaired vacuum (yrast) configuration. Also for this configuration we can, based on figure 10, distinguish three different regions. In the first region, to the left of the arrow marked gs, its structure is more or less similar to that of the g-configuration. In the second region, between the arrows gs and s3, it reminds more about the s-configuration, while in the third region, to the right of the arrow s3, it has a structure similar to that of the third configuration. The transition between the different regions is very gradual and does not give rise to any irregularities in the unpaired yrast line. The exact position of the arrows is therefore somewhat arbitrary.

Above the arrow s3 we must in fact identify the unpaired vacuum as the third configuration, although this configuration cannot be constructed

in a well-defined way from non-interacting levels when $\Delta=0$. It can however be constructed using the interacting levels, at least between the pseudo crossings (cf. table I). One then find that the self-consistent gap is zero for all frequencies (cf. table II), and consequently the self-consistent solution is a single-particle configuration. For low frequencies the situation is the same as the one we found for the s-configuration in subsection 7.4. When approaching $\Delta=0$ the structure of the wave function changes, and the self-consistent solutions, which we find do not contain the label components which we associate with the 3rd configuration, simply because there are no single-particle configurations with this label. For high frequencies, where the self-consistent solution corresponds to the unpaired vacuum, the label components appear in the wave function. This explains the large overlap seen in fig. 10 at high frequencies, and justifies the identification of the unpaired vacuum as the 3rd configuration.

One may get an idea of the pair correlation energy for each configuration by comparing its energy with the energy of the unpaired vacuum configuration for such values of the angular momentum where the two configurations have a similar structure. From fig. 9 we find a pairing energy of about $0.4 \hbar\omega_0$ for the g-configuration ($I \leq 6$) and $0.07 \hbar\omega_0$ for the s-configuration ($14 \leq I \leq 22$), while for the 3rd configuration the pairing energy is zero ($I \geq 24$).

It should be observed that the self-consistent pairing gap can be relatively large although the quasiparticle excitation energy, e , calculated in the rotating frame of reference (cf. table II), is high. Assume that the quasiparticle levels in fig. 3 were straight lines. Then, any configuration would have wave functions that are independent of ω . Its excitation energy at $\omega=0$ would be $e=e'+\omega i$ where i is the aligned angular momentum and e' the excitation energy relative to the g-configuration at the frequency ω . For the 2 quasiparticle configurations in table II ($\omega/\omega_0=0.02$) e lies between 2Δ and 4Δ , and one sees by analyzing these wave functions that they in fact are linear combinations of a few of the lowest 2 quasiparticle configurations at $\omega=0$. For the configuration [a,b,c,d] e' is not higher than for [e,f] while e due to the large alignment is considerably larger than 4Δ , underlining the 4 quasiparticle character of this configuration for which $\Delta_{s,c.}=0$. The yrast line is built up by a series of configurations with increasing aligned angular momentum and consequently increasing values of e . To

express the yrast configuration in terms of non-rotating quasiparticle configurations one has to use components containing an increasing number of excited quasiparticles, leading to a breakdown of pairing. Other configurations carrying no or very little aligned angular momentum can also at high frequencies be expressed in terms of the low-lying $\omega=0$ and 2 quasiparticle configurations only. Therefore the pair correlations will remain as it does for the g- and s-configurations shown in fig. 5. Although the presence of the core will modify the pairing properties of these configurations it would be very interesting to see experimentally if e.g. the continuation of the g-band above the first backbending still has a large pairing gap. The observation of a backbending within this band for ^{160}Yb at $\hbar\omega \approx 0.36$ MeV ($I \approx 14$) by Riedinger et al. ²⁶⁾ is interpreted as being caused by the pseudo crossing at ω_2^1 in fig. 3. This indicates the presence of strong pair correlations, in the absence of which this crossing would not appear and no irregularities should be expected.

10. SUMMARY

The results obtained in this paper are exclusively based on an $i_{13/2}^-$ model. We have, however, adjusted the parameters of the model in such a way, that we, when a comparison is possible, qualitatively reproduce the results found in full scale calculations. We give below a summary of the most important results, which we believe are representative also for realistic calculations.

- We have shown that it is possible to construct a set of non-interacting quasiparticle levels, which can be used in self-consistent calculations. The computation of these levels is in most cases relatively simple, and can be performed also in realistic calculations without any essential increase of the computation time.
- By using the non-interacting levels one avoids the spurious effects, which are connected with the pseudo level crossing, and which are the major drawback in cranked HFB-calculations. One obtains however always sharply crossing rotational bands. In realistic calculations it is therefore only possible to get a good agreement with experiment if the interaction between the experimental bands are very weak.

- The quasiparticle energy diagrams are indispensable for classifying different quasiparticle configurations, and for predicting when bandcrossings will appear. The results obtained in HFB-calculations using the interacting levels can easily be understood from the diagrams and the properties of the non-interacting configurations.
- Particle number projection causes always an increase of the self-consistent pairing gap. This effect can be understood as a result of the increasing impurity in particle number when Δ increases.
- Within a given non-interacting configuration, $\Delta_{s.c.}$ changes always slowly with the frequency. Along the yrast line, all important changes in $\Delta_{s.c.}$ are due to rotational alignment of individual pairs of quasiparticles connected with the configuration changes (bandcrossings).
- The investigation of the wave functions gives a very rich and normally easily interpreted information about the structure of the excited configurations. One of the most important features is that a label, i.e. certain typical components in the wave function, can be assigned to each configuration. The label is insensitive to changes in Δ except in the limit $\Delta \rightarrow 0$.

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TABLE CAPTIONS

Table 1. The correspondence between configurations constructed from the interacting levels (fig. 2) and the non-interacting levels (fig. 3) is shown. Between two "crossings" ω_1 , ω_2' etc. an interacting configuration, marked with letters to the left, corresponds to a non-interacting configuration as shown to the right. A configuration is specified by writing in parentheses those of the levels -d, -c, -b, -a, a, b, c, d (or -4, -3, -2, -1, 1, 2, 3, 4) that are filled. Lower lying levels (-e, -f, ... or -5, -6, ...) are always filled, higher lying levels (e, f, ... or 5, 6, ...) always free.

Table II. The left part of the table shows the self-consistent pairing gap and the aligned angular momentum calculated before ($\Delta_{s.c.}^{u.p.}$ and $i_{s.c.}^{u.p.}$) and after ($\Delta_{s.c.}^p$ and $i_{s.c.}^p$) particle number projection for some low-lying configurations. The right part of the table shows the aligned angular momentum i , the excitation energy e' and the quantity $e' + \omega i$, discussed in section 9. They are all calculated for $\Delta = 0.15 \hbar \omega_0$, which is the value used in figs. 2 and 3. The configuration labels indicate the levels with positive energy that are filled. All values given in this table are calculated for $\omega/\omega_0 = 0.02$.

Table III. Wave functions of the particle number projected $N=6$ g- and s-configurations. The table shows only the main components, which, except for the largest Δ -values, account for more than 90% of the total wave function. All wave functions are calculated for $\omega/\omega_0 = 0.01$, which is the frequency used in fig. 6.

Configuration	$\omega < \omega_1$	$\omega_1 < \omega < \omega_2^I$	$\omega_2^I < \omega < \omega_2^{II}$	$\omega_2^{II} < \omega < \omega_3$	$\omega > \omega_3$
$[-a, -b, -c, -d]$ vacuum	$[-1, -2, -3, -4]$ ground	$[1, 2, -3, -4]$ Stockholm	$[1, 2, -3, -4]$ Stockholm	$[1, 2, -3, -4]$ Stockholm	$[1, 2, 3, 4]$ 3rd
$[a, b, -c, -d]$ lowest 2 q.p.	$[1, 2, -3, -4]$ Stockholm	$[-1, -2, -3, -4]$ ground	$[-1, 2, 3, -4]$ 4th	$[1, 2, 3, 4]$ 3rd	$[1, 2, -3, -4]$ Stockholm
$[-a, b, c, -d]$	$[-1, 2, 3, -4]$ 4th	$[-1, 2, 3, -4]$ 4th	$[-1, -2, -3, -4]$ ground	$[1, -2, -3, 4]$ 5th	$[1, -2, -3, 4]$ 5th (A)
$[a, -b, -c, d]$	$[1, -2, -3, 4]$ 5th	$[1, -2, -3, 4]$ 5th	$[1, 2, 3, 4]$ 3rd	$[-1, 2, 3, -4]$ 4th	$[-1, 2, 3, -4]$ 4th (B)
$[-a, -b, c, d]$	$[-1, -2, 3, 4]$ 6th	$[1, 2, 3, 4]$ 3rd	$[1, -2, -3, 4]$ 5th	$[-1, -2, -3, -4]$ ground	$[-1, -2, 3, 4]$ 6th (C)
$[a, b, c, d]$ lowest 4 q.p.	$[1, 2, 3, 4]$ 3rd	$[-1, -2, 3, 4]$ 6th	$[-1, -2, 3, 4]$ 6th	$[-1, -2, 3, 4]$ 6th	$[-1, -2, -3, -4]$ ground (D)

Note: slightly above ω_3 the configurations having the levels -1 and/or -2 filled meet further crossings. At ω_4^I the levels -2 and 5 cross and at ω_4^{II} the levels -1 and 6 cross. Including also the levels -6, -5, 5 and 6 we get

- (A) $[-a, b, c, -d]$ corresponds to $[1, 2, -3, 4, 5, -6]$ for $\omega > \omega_4^I$
- (B) $[a, -b, -c, d]$ corresponds to $[1, 2, 3, -4, -5, 6]$ for $\omega > \omega_4^{II}$
- (C) $[-a, -b, c, d]$ corresponds to $[-1, 2, 3, 4, 5, -6]$ for $\omega_4^I < \omega < \omega_4^{II}$ and to $[1, 2, 3, 4, 5, 6]$ for $\omega > \omega_4^{II}$
- (D) $[a, b, c, d]$ corresponds to $[-1, 2, -3, -4, 5, -6]$ for $\omega_4^I < \omega < \omega_4^{II}$ and to $[1, 2, -3, -4, 5, 6]$ for $\omega > \omega_4^{II}$.

Similarly the continuation of the ground configuration becomes $[a, b, -c, d, e, -f]$ for $\omega_4^I < \omega < \omega_4^{II}$ and $[a, b, -c, -d, e, f]$ for $\omega > \omega_4^{II}$.

Configuration	Unprojected; $\Delta=0.15 \text{ } \mathcal{H}_{\omega_0}$				Projected; $\Delta=0.15 \text{ } \mathcal{H}_{\omega_0}$					
	$\text{u.p. } \Delta_{\text{S.C.}}$	$\text{i u.p. }_{\text{S.C.}}$	$\text{P. } \Delta_{\text{S.C.}}$	$\text{i P. }_{\text{S.C.}}$	i	e'	$\text{e' + } \omega \text{i}$	i	e'	$\text{e' + } \omega \text{i}$
[vac]	0.34	0	0.37	0	0	0	0	0	0	0
[a,b]	0.14	8.67	0.24	9.78	8.90	0.246	0.424	8.92	0.338	0.516
[b,c]	0.14	7.90	0.20	8.87	8.03	0.319	0.480	8.04	0.419	0.579
[a,d]	0.13	5.83	0.18	6.62	6.23	0.333	0.457	6.10	0.437	0.559
[c,d]	0.17	6.34	0.23	7.11	6.08	0.414	0.536	5.71	0.536	0.651
[e,f]	0.18	0.73	0.23	0.68	0.72	0.552	0.567	0.50	0.680	0.690
[a,b,c,d]	0*	7.80*	0*	7.80*	13.80	0.552	0.828	14.90	0.769	1.067

* The selfconsistent ($\Delta_{\text{s.c.}}=0$) wave function of the configuration [a,b,c,d] is structurally completely different from the wave function of the same configurationcalculated at $\Delta=0.15 \text{ } \mathcal{H}_{\omega_0}$, cf. subsection 7.4 and section 9.

g-configuration

$\Delta/\hbar\omega_0$	$ \bar{5} \bar{3} 1 \bar{5} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{3}, \bar{2}\rangle$	$ \bar{7} \bar{3} 1 \bar{7} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	$ \bar{7} \bar{5} 1 \bar{7} \bar{5} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	$ \bar{7} \bar{5} 3 \bar{7} \bar{5} \bar{3}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	$ \bar{9} \bar{3} 1 \bar{9} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$
0.30	0.6695	-0.4154	0.3122	-0.2746	0.2322
0.20	0.7949	-0.3898	0.2645	-0.2249	0.1787
0.10	0.9418	-0.2279	0.1326	-0.1078	0.0810
0.05	0.9691	-0.0559	0.0422	-0.0334	0.0251

s-configuration

$\Delta/\hbar\omega_0$	$ \bar{5} \bar{3} 1 \bar{5} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	$ \bar{7} \bar{3} 1 \bar{7} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	$ \bar{5} \bar{3} 1 \bar{7} \bar{5} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	$ \bar{7} \bar{5} 1 \bar{5} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	Label	
					$ \bar{5} \bar{3} 1 \bar{7} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$	$ \bar{7} \bar{3} 1 \bar{5} \bar{3} \bar{1}\rangle$ $ \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}, \bar{2}\rangle$
0.30	0.4006	0.4272	0.1416	0.1518	0.4131	0.4181
0.20	0.4310	0.4604	0.1415	0.1486	0.4578	0.4613
0.10	0.3377	0.4960	0.1510	0.1569	0.5119	0.5153
0.05	0.1260	0.4894	0.1715	0.1784	0.5585	0.5638
0.02	-0.1200	0.4037	0.1956	0.2074	0.5826	0.5974
0.01	-0.2093	0.3457	0.2022	0.2211	0.5773	0.6099
0.00	-0.2057	0.1927	0.0063	0.3243	0.0450	0.8806

FIGURE CAPTIONS

Fig. 1. The aligned angular momentum i of the s -configuration as a function of the pairing gap Δ . The dashed curve is calculated with the $i_{13/2}$ model used in this paper assuming 6 particles in the $i_{13/2}$ shell. The solid line is taken from a realistic calculation ⁹⁾ for ^{164}Er , in which the number of particles in the $i_{13/2}$ shell is close to 6. The experimentally estimated values of i for ^{164}Er and ^{166}Yb are also shown (from ref. ¹¹⁾). These results indicate that the pairing gap is large, around $0.1 \hbar\omega_0$, for the s -configuration. A similar theoretical value (Δ_s) is obtained for the s -band of ^{164}Er in ref. ¹¹⁾ after particle number projection. It is only slightly smaller than the gap, Δ_g , calculated for the g -band. All values shown in this figure are relevant for the experimental backbending frequency.

Fig. 2. Quasiparticle energies of the $i_{13/2}$ shell as a function of the rotational frequency calculated with $\Delta=0.15 \hbar\omega_0$ and $\lambda=6.50 \hbar\omega_0$ ($e_0=6.655 \hbar\omega_0$ in eq. (2.2)). Levels having the signature $\alpha=1/2$ are drawn with solid lines, those having $\alpha=-1/2$ with dashed lines. The pseudo crossings discussed in the text are indicated (only for the $\alpha=1/2$ levels) with arrows.

Fig. 3. Same as fig. 2, but after the interaction at the pseudo crossings has been eliminated.

Fig. 4. Single-particle energies of the $i_{13/2}$ shell as functions of the rotational frequency. Solid lines denote $\alpha=1/2$ and dashed lines $\alpha=-1/2$. The energies have been calculated using $e_0=0$ (eq. (2.2)).

Fig. 5. The self-consistent pairing gap calculated before (solid lines) and after (dashed lines) particle number projection. The dot-dashed lines show the position of those pseudo crossings, which are indicated in figs. 2 and 3. Notice that the crossing frequencies depend strongly on Δ and that ω_2' and ω_2'' do not influence the s -configuration. Since the non-interacting quasiparticle levels has been used, no irregularities are observed at the crossing frequencies.

Fig. 6. The upper part shows the particle number projected energies (solid lines with figures indicating the particle number) and the unprojected energy (dot-dashed line). The weighted average of the

projected energies is also shown (dashed line). It can be calculated from the unprojected wave function as the expectation value of the Hamiltonian of eq. (5.1). The lower part of the figure shows the probability, n , for different particle numbers in the unprojected wave function. The rotational frequency is $\omega/\omega_0=0.01$ and λ has been chosen so as to give $\langle N \rangle=6$. In eq. (2.2) $e_0=0.2 \hbar \omega_0$ has been used (see comments in the text).

Fig. 7. The energy $E'_N(\Delta, \omega)$, calculated for the vacuum configuration using the interacting levels without particle number projection. Of the dashed lines the one to the left shows the position of the pseudo crossing at ω_1 and the one to the right the position of the pseudo crossing at ω_3 . The dot-dashed line shows the self-consistent non-zero values $\Delta_{s.c.}$. A closer inspection of the figure shows that in cases where three values of $\Delta_{s.c.}$ can be found for the same frequency, the smallest and the largest value correspond to a minimum while the intermediate value (near the ω_1 -line) corresponds to a maximum of $E'_N(\Delta, \omega)$.

Fig. 8. The self-consistent gap (Δ) of the vacuum configuration and the configuration $[a, b, -c, -d]$ calculated from the interacting levels without particle number projection. The dotted lines show the gap of the g- and the s-configurations (cf. fig. 5) calculated from the non-interacting levels. We have also included parts of the $\Delta_{s.c.}$ curves for the configurations $[-a, b, c, -d]$ and $[-a, -b, c, d]$ to show that these configurations build up parts of the g-configuration between ω_2' and ω_2'' and between ω_2'' and ω_3 respectively.

Fig. 9. The rotational energy, E , versus the angular momentum, I , for the three configurations (g-, s- and 3rd) building up the lowest part of the yrast line. The figure also shows the unpaired yrast configuration, $[A, B, C, \bar{A}, \bar{B}, \bar{C}]$ (cf. fig. 4), which above the arrow s3 goes over into the 3rd configuration. The energy is calculated by adding a rotor to the $i_{13/2}$ shell:

$$E = \epsilon + \omega \langle J_x \rangle_{13/2} + 0.5 \mathcal{J}_C J^2$$

$$I = \omega \mathcal{J}_C + \langle J_x \rangle_{13/2}$$

where $\mathcal{J}_C = 60/\kappa$ as in ref. ¹²⁾. The energy ϵ is obtained as the

expectation value of the Hamiltonian of eq. (5.1) for the projected $N=6$ states.

Fig. 10. Overlap integrals for the particle number projected quasiparticle configurations g-, s- and 3 with the unpaired vacuum. To ensure that the quasiparticle configurations have their typical label we have chosen $\Delta=0.15 \hbar\omega_0$ for all three configurations. Although two of the quasiparticle configurations may both have a large overlap with the unpaired vacuum for a given frequency, their mutual overlap is always relatively small, cf. section 7.3.

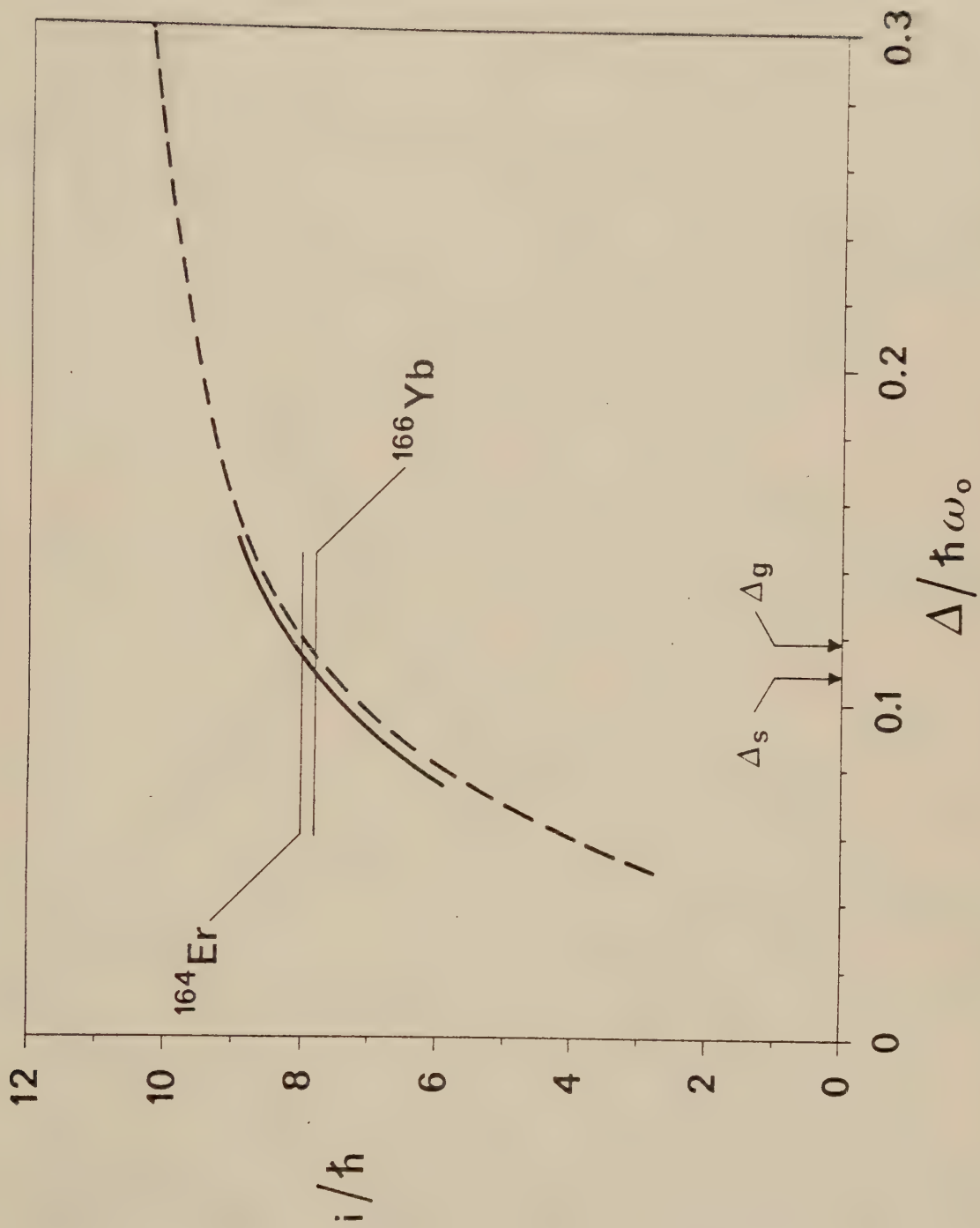


Fig. 1

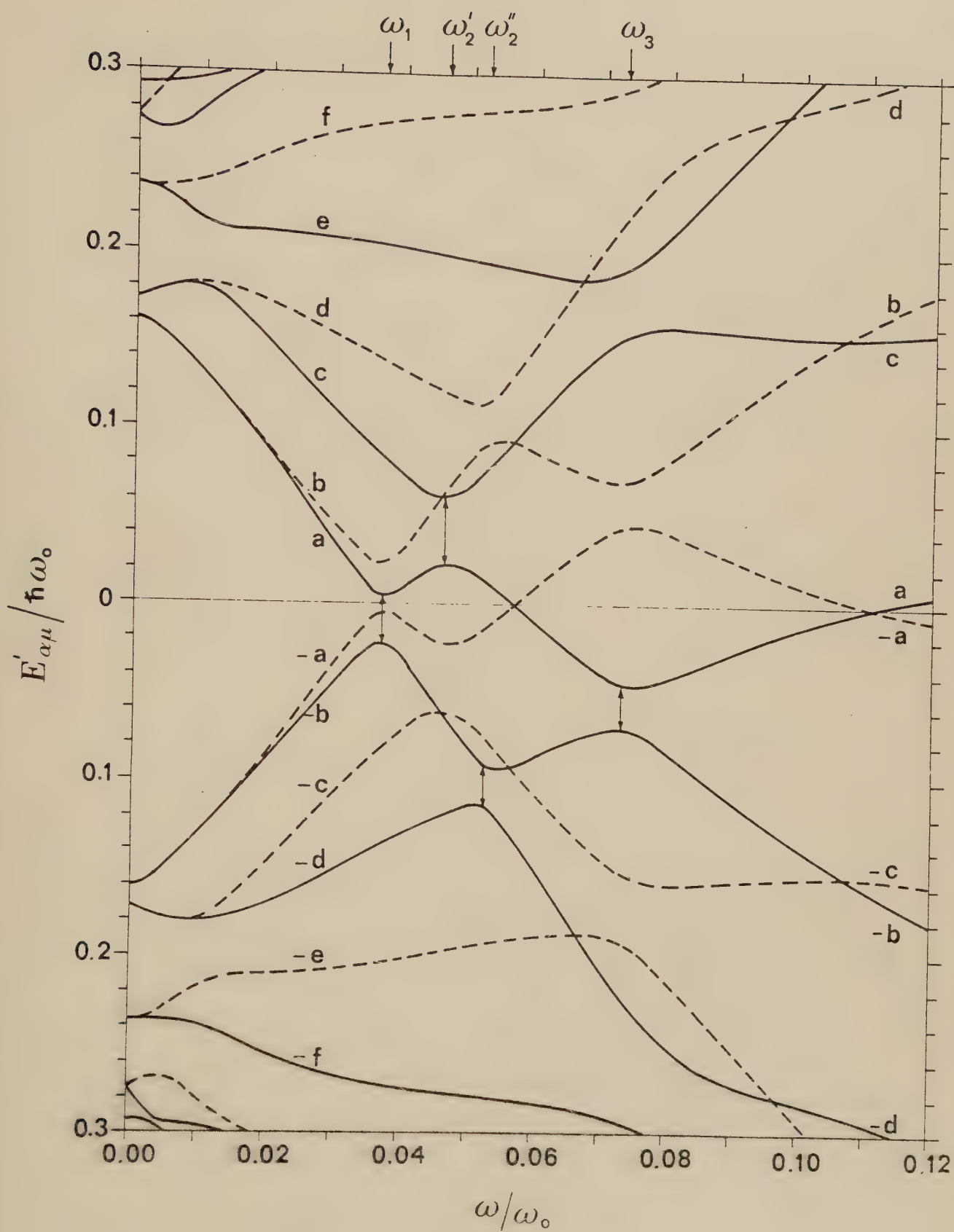


Fig. 2

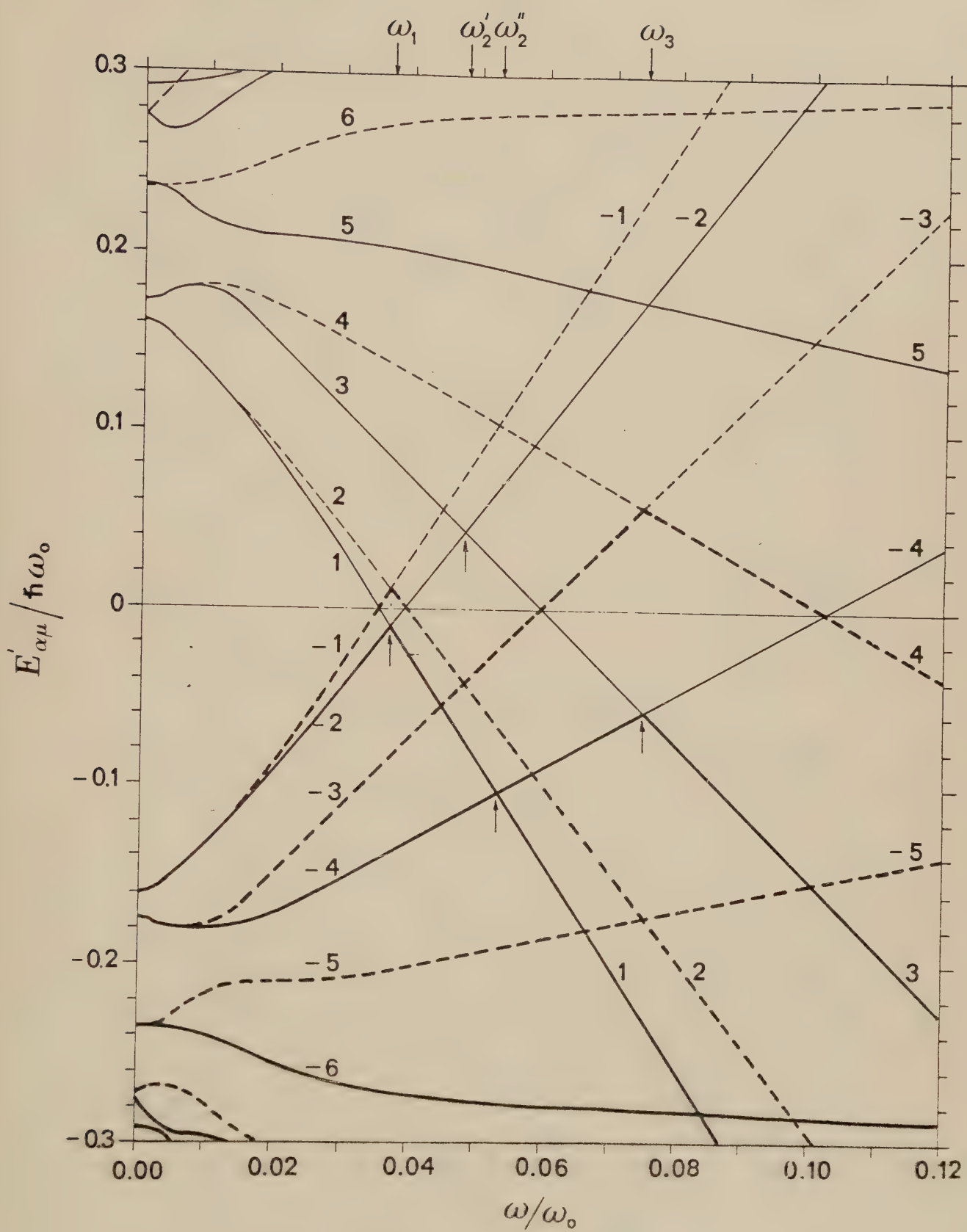


Fig. 3

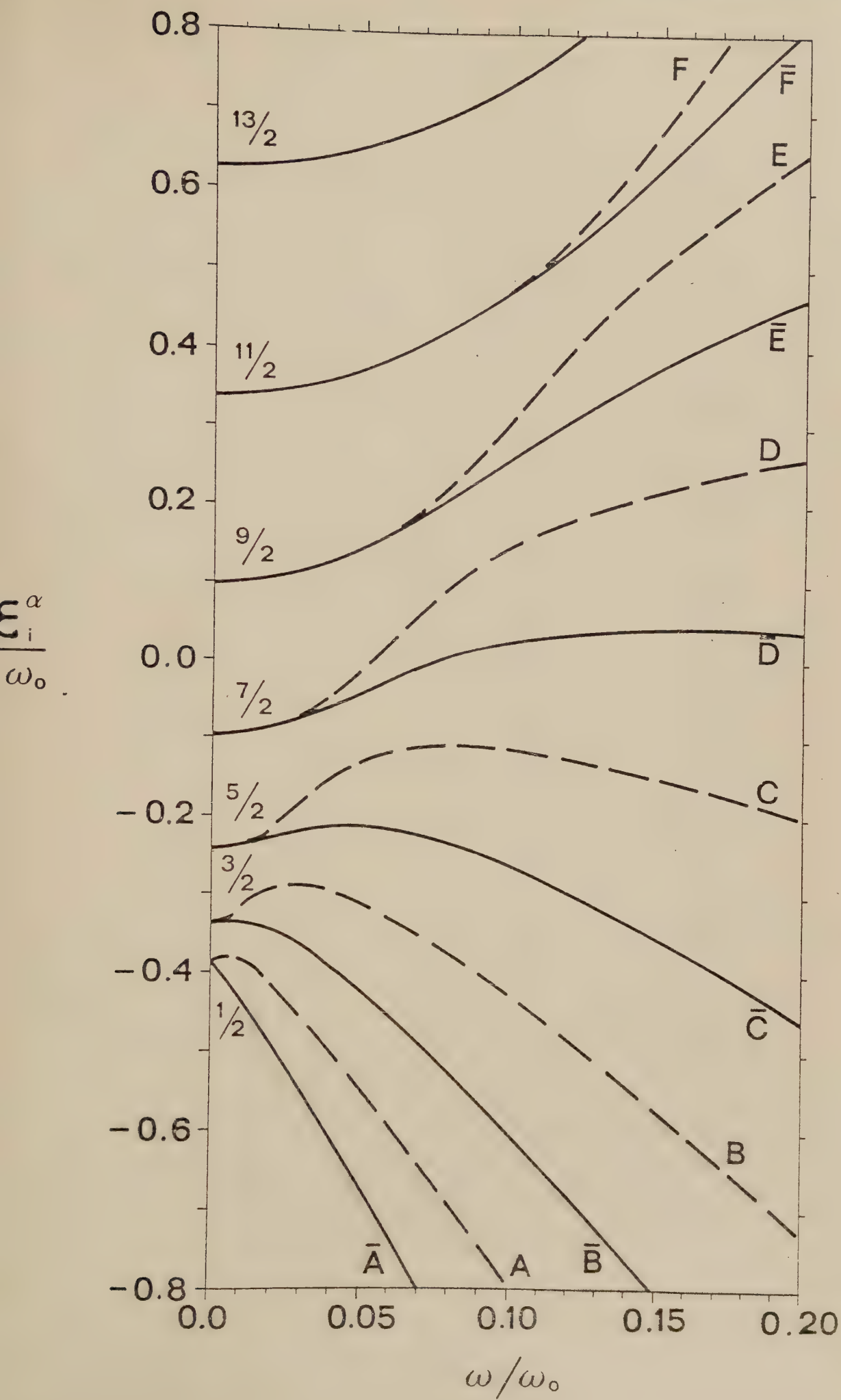


Fig. 4

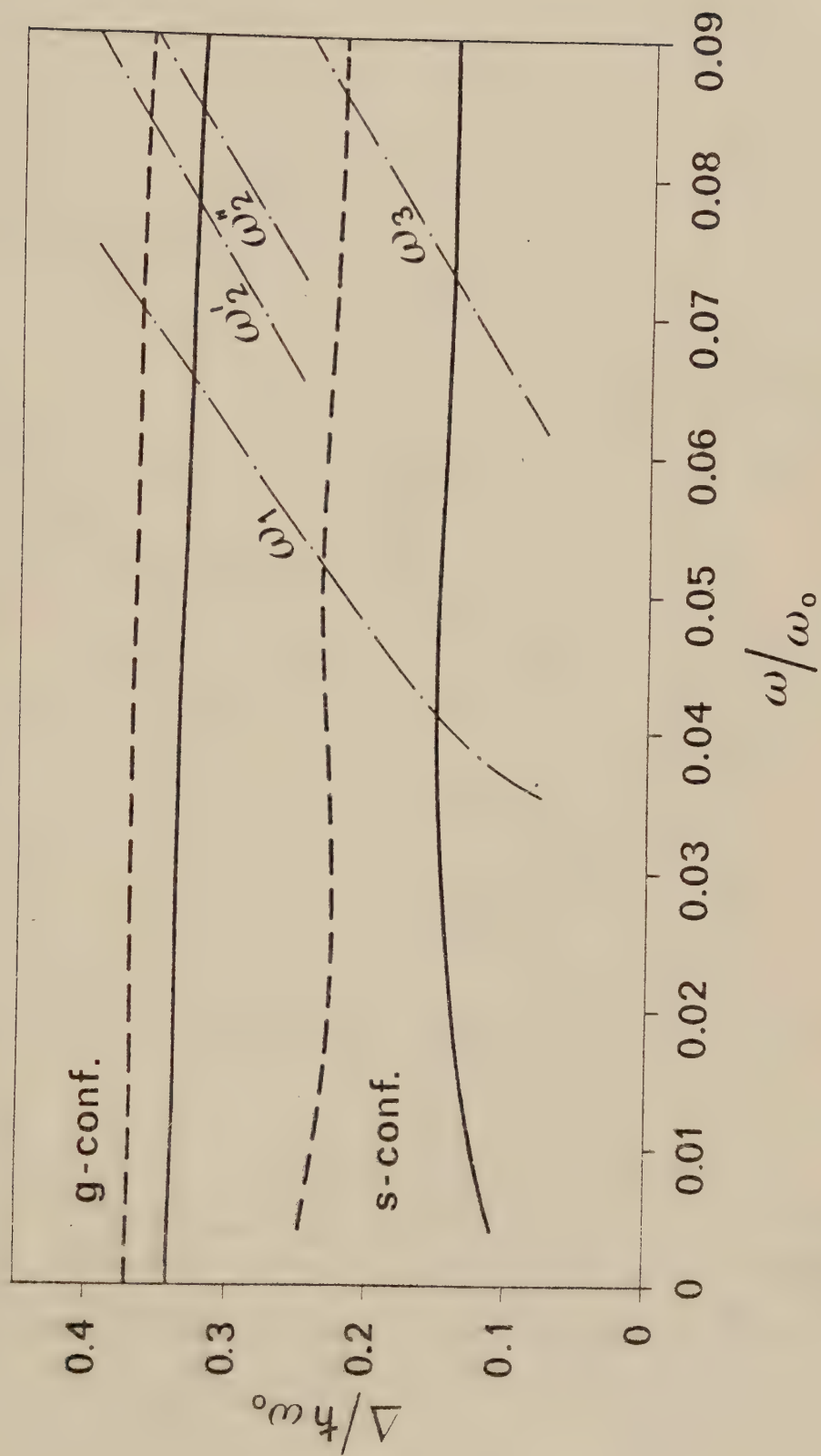


Fig. 5

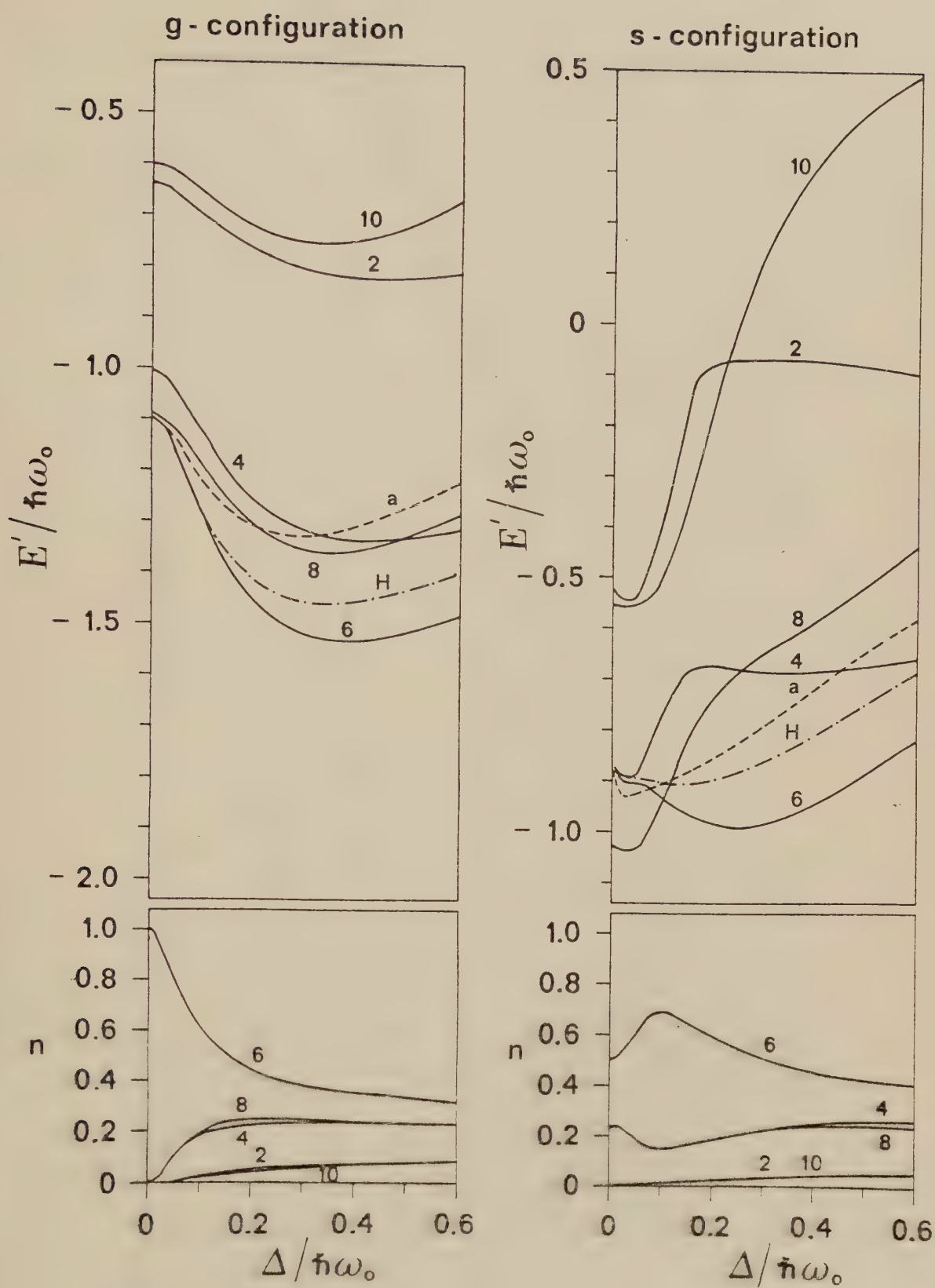


Fig. 6

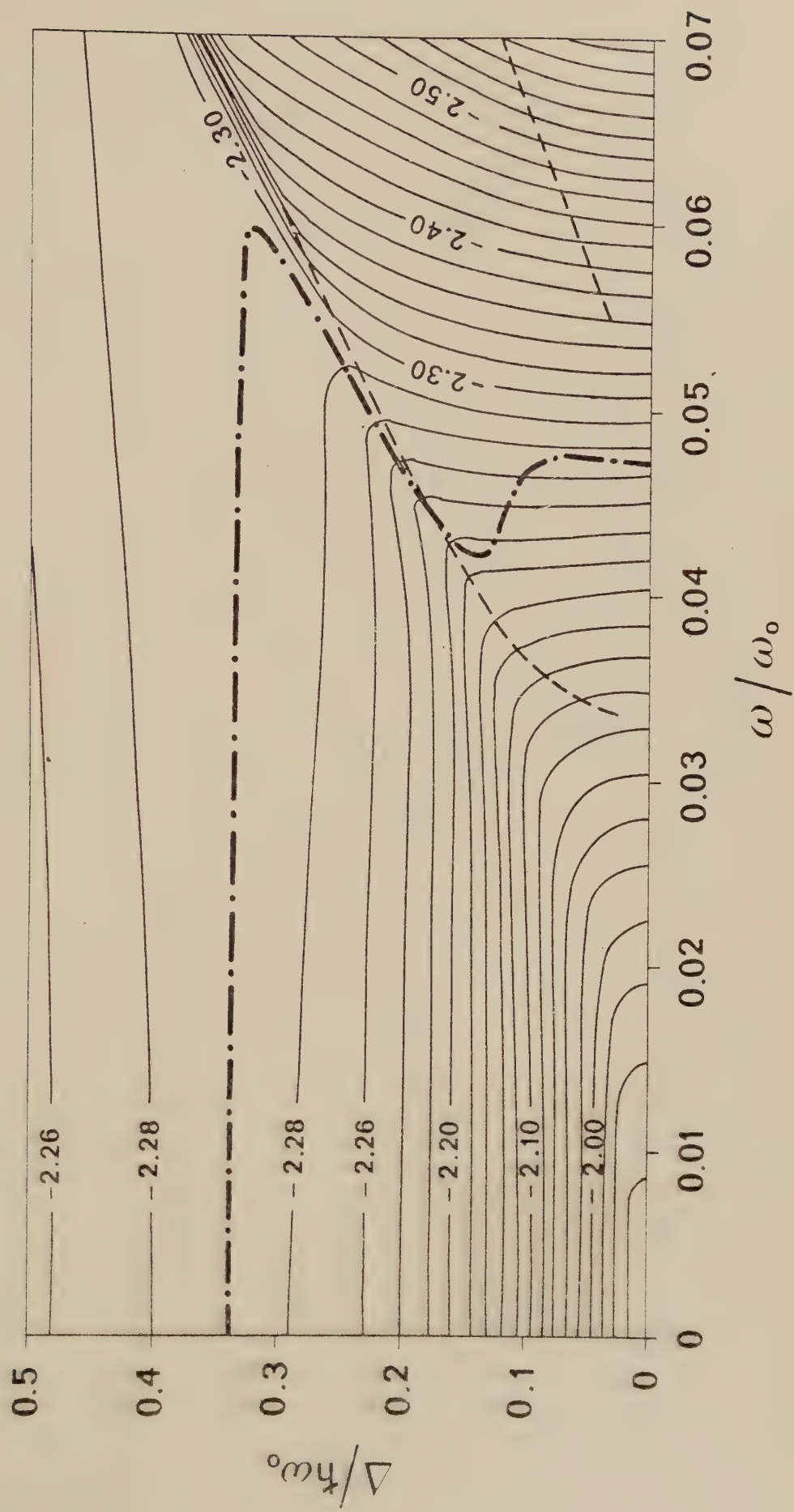


Fig. 7

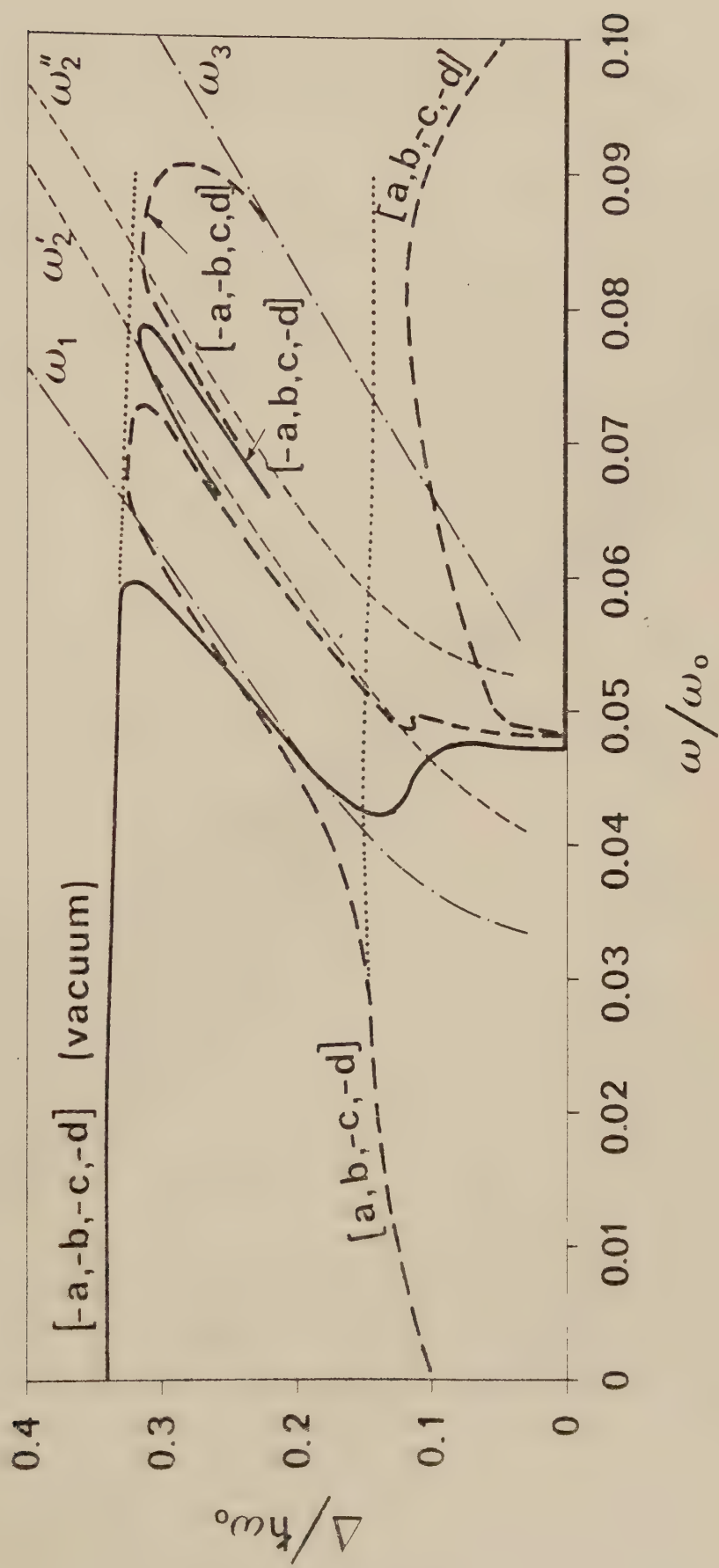


Fig. 8

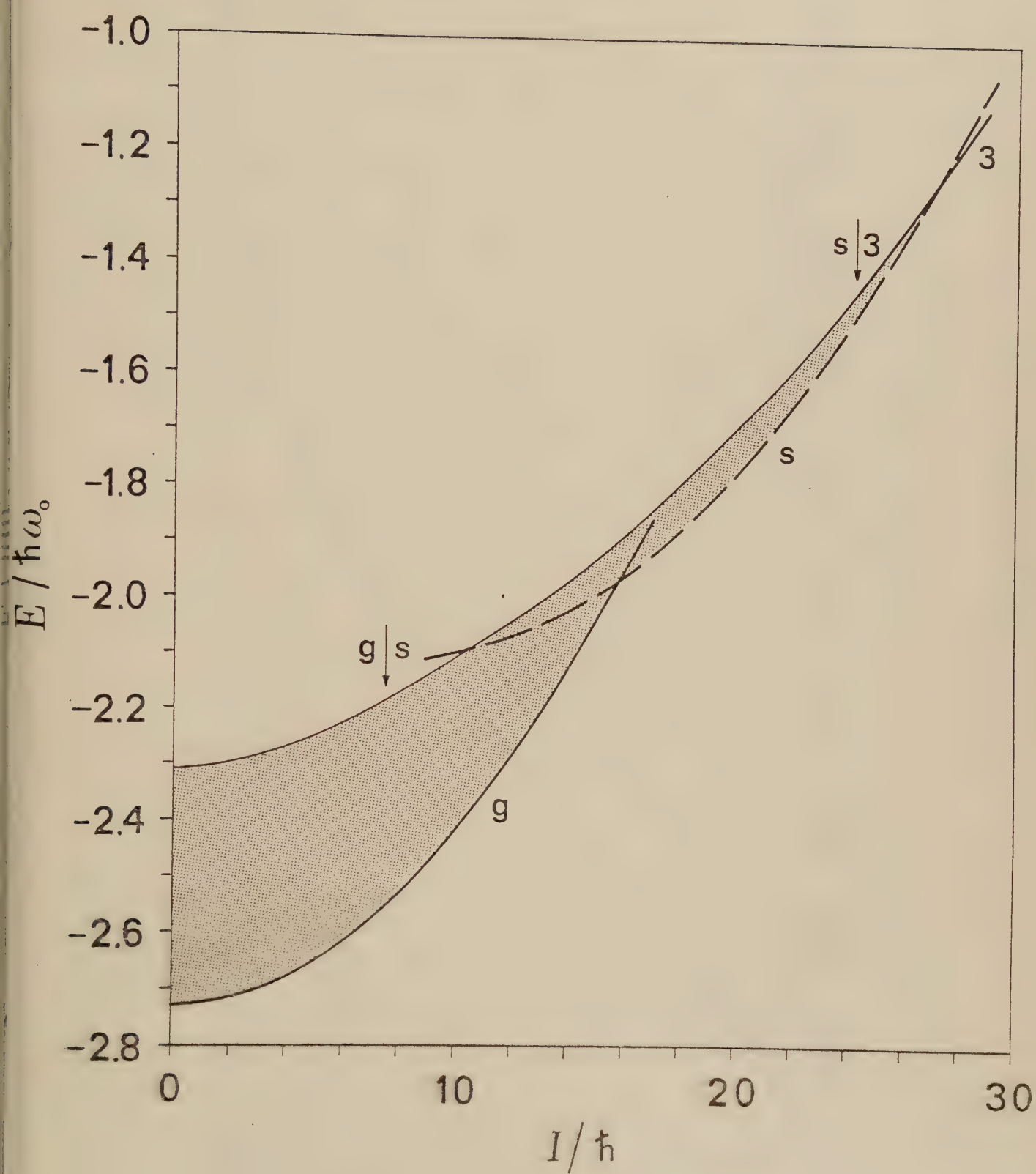


Fig. 9

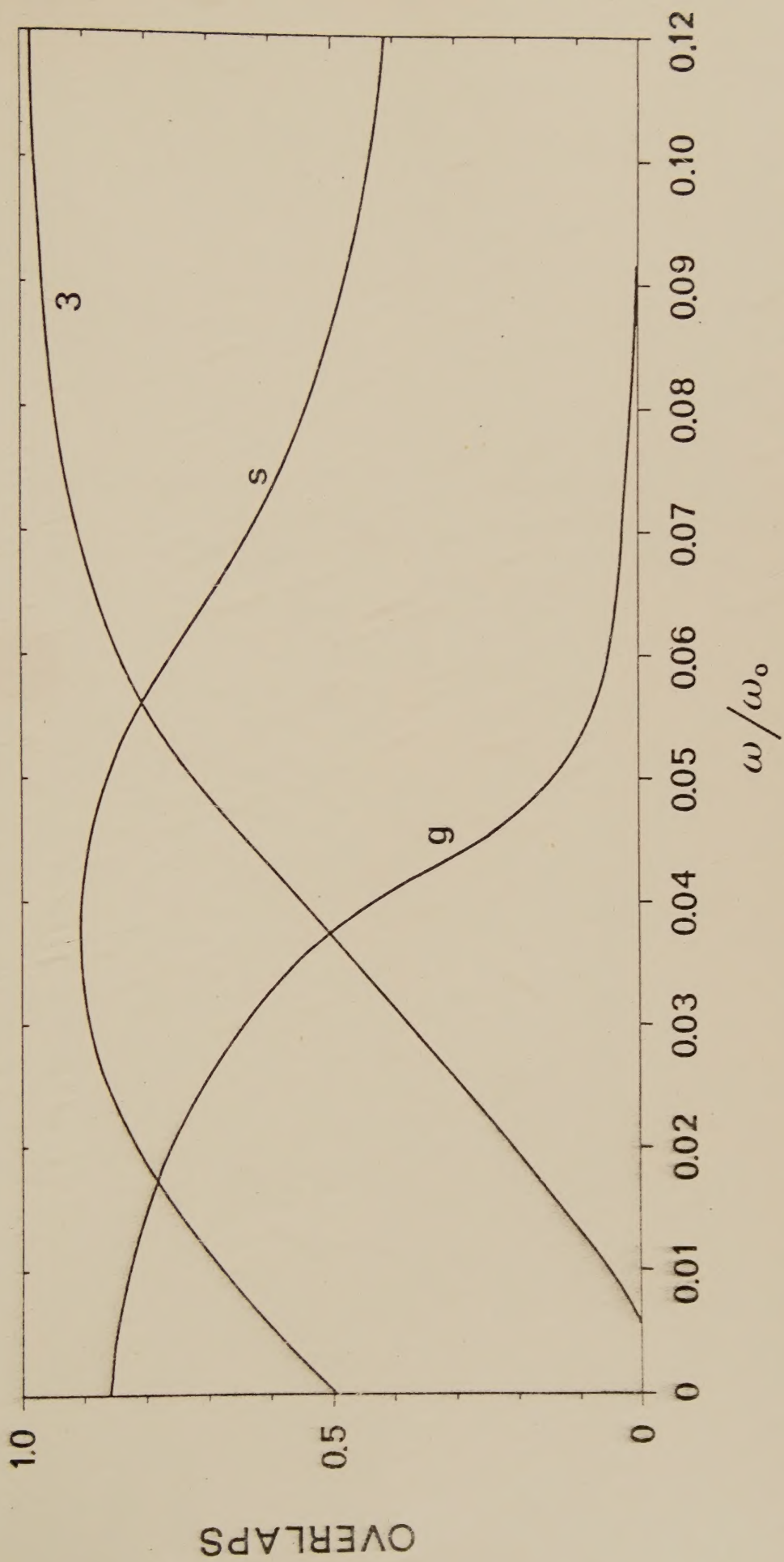


Fig. 10

